Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Infrared Photodissociation Spectroscopy of Heteronuclear Group 15 Metal–Iron Carbonyl Cluster Anions $A_mFe(CO)_n^-$ (A = Sb, Bi; m, n = 2, 3)

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Table S1 Symmetries, electronic states, and relative energies (ΔE, in kJ/mol, zero-point vibrational energies were included.) of the structures of $Sb_mFe(CO)_n^-$ (m, n = 2, 3) calculated at the B3LYP/SDD(Sb)/aug-cc-pVTZ(Fe, C, O), and BP86/SDD(Sb)/aug-cc-pVTZ(Fe, C, O) levels.

Isomer [a]	B3LYP		BP86	
	Sym.	ΔE	Sym.	ΔE
$Sb_2Fe(CO)_2^-$				
1a	C_{2v} ($^2A_1$)	0.0	C_{2v} ($^2A_1$)	0.0
1b	C_{2v} ($^4A_2$)	61.3	C_{2v} ($^4A_2$)	84.4
1c	C_{2v} ($^4B_2$)	67.4	C_{2v} ($^4B_2$)	96.4
1d	C_{2v} ($^2A_1$)	136.0	C_{2v} ($^2A_1$)	140.9
$Sb_3Fe(CO)_2^-$				
2a	C_s ($^3A''$)	0.0	C_s ($^3A''$)	16.2
2b	C_s ($^1A'$)	19.1	C_s ($^1A'$)	0.0
2c	C_s ($^1A'$)	62.0	C_s ($^1A'$)	41.5 (19*i*)
2d	C_{2v} ($^3B_1$)	67.7	C_{2v} ($^3B_1$)	69.3 (41*i*)
2e	C_2 (^3B)	118.9	C_2 (^3B)	142.2 (10*i*)
2f	C_s ($^3A'$)	131.4	C_s ($^3A'$)	167.7
2g	C_{2v} ($^3A_2$)	157.1	C_{2v} ($^3A_2$)	194.9
2h	C_s ($^1A'$)	169.9	C_s ($^1A'$)	142.8
$Sb_2Fe(CO)_3^-$				
3a	C_s ($^2A'$)	0.0	C_s ($^2A'$)	0.0 (15*i*)
3b	C_s ($^4A'$)	81.0	C_s ($^4A'$)	103.2
3c	C_s ($^4A''$)	85.4	C_s ($^4A''$)	104.7
3d	C_1 (^4A)	94.1	C_s ($^4A''$)	136.7 (5*i*)
3e	C_s ($^2A'$)	101.6	C_s ($^2A'$)	93.6

3f	C_{2v} ($^4A_1$)	142.6	C_{2v} ($^4A_1$)	140.2
$Sb_3Fe(CO)_3^-$				
4a	C_{3v} ($^1A_1$)	0.0	C_{3v} ($^1A_1$)	0.0
4b	C_s ($^3A'$)	106.4	C_s ($^3A'$)	136.5
4c	C_s ($^3A''$)	111.4	C_s ($^3A''$)	122.9
4d	C_s ($^1A'$)	142.5	C_s ($^1A'$)	132.4
4e	C_{2v} ($^3A_2$)	160.1	C_{2v} ($^3A_2$)	198.2
4f	C_s ($^3A''$)	185.6	C_s ($^3A''$)	187.8 (609*i*)
4g	C_1 (^3A)	198.4	C_1 (^3A)	201.8
4h	C_1 (^3A)	223.4	C_1 (^3A)	242.7
4i	C_s ($^1A'$)	243.5	C_s ($^1A'$)	250.0
4j	C_1 (^1A)	244.1	C_1 (^1A)	250.7
4k	C_1 (^3A)	252.2	C_1 (^3A)	270.3
4l	C_s ($^3A''$)	261.2	C_s ($^3A''$)	284.4

[a] Refer to the structures displayed in Fig. 6, 7, 8, and 9.

Table S2 Symmetries, electronic states, and relative energies (in kJ/mol, zero-point vibrational energies were included.) of the structures of $Bi_mFe(CO)_n^-$ (m = 2, 3; n = 2, 3) calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O), and BP86/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) levels.

Isomer [a]	B3LYP		BP86	
	Sym.	ΔE	Sym.	ΔE
$Bi_2Fe(CO)_2^-$				
1a’	C_{2v} ($^2A_1$)	0.0	C_{2v} ($^2A_1$)	0.0
1b’	C_{2v} ($^4B_2$)	60.6	C_{2v} ($^4B_2$)	89.2
1c’	C_{2v} ($^4A_2$)	63.8	C_{2v} ($^4A_2$)	86.8
1d’	C_{2v} ($^2A_1$)	136.6	C_{2v} ($^2A_1$)	144.9
$Bi_3Fe(CO)_2^-$				
2a’	C_1 (^3A)	0.0	C_1 (^3A)	13.4
2b’	C_s ($^1A’$)	23.9	C_s ($^1A’$)	0.0
2c’	C_1 (^3A)	42.0	C_1 (^3A)	56.8
2d’	C_{2v} ($^3B_1$)	75.2	C_{2v} ($^3B_1$)	71.9 (28*i*)
2e’	C_{2v} ($^3B_2$)	130.3	C_{2v} ($^3B_2$)	149.0 (12*i*)
2f’	C_s ($^1A’$)	197.5	C_s ($^1A’$)	164.8
$Bi_2Fe(CO)_3^-$				
3a’	C_s ($^2A’$)	0.0	C_1 (^2A)	0.0
3b’	C_s ($^4A’$)	76.6	C_s ($^4A’$)	93.6
3c’	C_s ($^4A’’$)	77.5	C_s ($^4A’’$)	94.6
3d’	C_1 (^4A)	86.0 (4*i*)	C_1 (^4A)	129.2
3e’	C_s ($^2A’$)	104.0	C_s ($^2A’$)	98.5
$Bi_3Fe(CO)_3^-$				
4a’	C_{3v} ($^1A_1$)	0.0	C_{3v} ($^1A_1$)	0.0

4b’	C_1 (^{3}A)	90.7	C_1 (^{3}A)	122.0
4c’	C_s (^{3}A’’)	111.0	C_s (^{3}A’’)	119.8
4d’	C_s (^{1}A’)	129.7	C_s (^{1}A’)	120.9
4e’	C_s (^{3}A’’)	155.7	C_s (^{3}A’’)	195.1
4f’	C_s (^{3}A’’)	178.7	C_s (^{3}A’’)	188.9
4g’	C_1 (^{3}A)	190.7	C_1 (^{3}A)	188.8
4h’	C_s (^{1}A’)	257.6	C_s (^{1}A’)	260.8 (2*i*)

[a] Refer to the structures displayed in Fig. S1, S2, S3, and S4.

Table S3 The Cartesian coordinates (Å) of the structures of $Sb_mFe(CO)_n^-$ (m, n = 2, 3) optimized at the B3LYP/SDD(Sb)/aug-cc-pVTZ(Fe, C, O), and BP86/SDD(Sb)/aug-cc-pVTZ(Fe, C, O) levels, respectively.

Isomer		B3LYP			BP86		
$Sb_2Fe(CO)_2^-$							
1a	Fe	0.00000000	0.00000000	1.17488500	0.00000000	0.00000000	1.16148600
	C	0.00000000	1.38410800	2.28050900	0.00000000	1.37344300	2.26727400
	C	0.00000000	-1.38410800	2.28050900	0.00000000	-1.37344300	2.26727400
	O	0.00000000	2.26673000	3.03756100	0.00000000	2.25653100	3.04829300
	O	0.00000000	-2.26673000	3.03756100	0.00000000	-2.25653100	3.04829300
	Sb	0.00000000	1.33434200	-1.04425600	0.00000000	1.34243700	-1.04096700
	Sb	0.00000000	-1.33434200	-1.04425600	0.00000000	-1.34243700	-1.04096700
1b	Fe	0.00000000	0.00000000	1.21431300	0.00000000	0.00000000	1.17488400
	C	0.00000000	1.53888900	2.26727800	0.00000000	1.45972200	2.25258700
	C	0.00000000	-1.53888900	2.26727800	0.00000000	-1.45972200	2.25258700
	O	0.00000000	2.53259000	2.85932700	0.00000000	2.39171700	2.97026100
	O	0.00000000	-2.53259000	2.85932700	0.00000000	-2.39171700	2.97026100
	Sb	-1.34001000	0.00000000	-1.02479100	-1.34837800	0.00000000	-1.03041400
	Sb	1.34001000	0.00000000	-1.02479100	1.34837800	0.00000000	-1.03041400
1c	Fe	0.00000000	0.00000000	1.29717700	0.00000000	0.00000000	1.21924300
	C	0.00000000	1.67134400	2.05745800	0.00000000	1.56150300	2.10244800
	C	0.00000000	-1.67134400	2.05745800	0.00000000	-1.56150300	2.10244800
	O	0.00000000	2.72122000	2.53999200	0.00000000	2.57926200	2.68736000
	O	0.00000000	-2.72122000	2.53999200	0.00000000	-2.57926200	2.68736000
	Sb	0.00000000	1.37519100	-0.97113700	0.00000000	1.40320000	-0.97968100
	Sb	0.00000000	-1.37519100	-0.97113700	0.00000000	-1.40320000	-0.97968100
1d	Fe	0.00000000	0.00000000	-2.19037900	0.00000000	0.00000000	-2.17308100
	Sb	0.00000000	0.00000000	0.28306900	0.00000000	0.00000000	0.24645000
	Sb	0.00000000	0.00000000	2.86867200	0.00000000	0.00000000	2.83989600
	C	0.00000000	1.43357200	-3.27583600	0.00000000	1.46260700	-3.17851000
	C	0.00000000	-1.43357200	-3.27583600	0.00000000	-1.46260700	-3.17851000
	O	0.00000000	-2.31755000	-4.02993100	0.00000000	-2.37730300	-3.92258600
	O	0.00000000	2.31755000	-4.02993100	0.00000000	2.37730300	-3.92258600
$Sb_3Fe(CO)_2^-$							
2a	Sb	0.47147400	-1.03708600	1.42602900	0.47851000	-1.02226700	1.43602900
	Sb	0.47147400	-1.03708600	-1.42602900	0.47851000	-1.02226700	-1.43602900
	Sb	-1.82743000	-0.00231200	0.00000000	-1.82714300	-0.02552200	0.00000000
	Fe	0.47147400	1.24178900	0.00000000	0.47851000	1.22288900	0.00000000
	C	2.19956500	1.60335200	0.00000000	2.18159700	1.63303400	0.00000000
	C	-0.25031200	2.88695400	0.00000000	-0.28405100	2.83244300	0.00000000
	O	3.32857100	1.87411000	0.00000000	3.31378100	1.96037500	0.00000000
	O	-0.68421900	3.95992800	0.00000000	-0.74506600	3.91273500	0.00000000
2b	Sb	0.32254100	-1.16101700	1.43769600	0.32729000	-1.15832800	1.44497500
	Sb	0.32254100	-1.16101700	-1.43769600	0.32729000	-1.15832800	-1.44497500
	Sb	-1.60708500	0.39814500	0.00000000	-1.61154600	0.37033500	0.00000000
	Fe	0.89223800	1.01219000	0.00000000	0.88445900	1.02165200	0.00000000
	C	0.92371100	2.12467000	1.35443500	0.92176400	2.14120400	1.33426500
	C	0.92371100	2.12467000	-1.35443500	0.92176400	2.14120400	-1.33426500

	O	0.92371100	2.89408600	2.22310400	0.92176400	2.93781000	2.20390900
	O	0.92371100	2.89408600	-2.22310400	0.92176400	2.93781000	-2.20390900
2c	Sb	-1.14083500	-1.43992000	0.00000000	-1.03979700	-1.53548700	0.00000000
	Sb	0.77409500	-0.30267500	1.74798100	0.73667400	-0.24625600	1.80375500
	Sb	0.77409500	-0.30267500	-1.74798100	0.73667400	-0.24625600	-1.80375500
	Fe	-0.12008300	1.14271500	0.00000000	-0.13988100	1.12828000	0.00000000
	C	-1.75153200	1.83967800	0.00000000	-1.76740000	1.81658400	0.00000000
	C	0.77409500	2.65336300	0.00000000	0.73667400	2.63096100	0.00000000
	O	1.34263400	3.66352800	0.00000000	1.31299400	3.65757800	0.00000000
	O	-2.81617600	2.29146300	0.00000000	-2.84923000	2.26835300	0.00000000
2d	Sb	2.23847800	0.00000000	0.11875700	2.20432700	0.00000000	0.04637700
	Sb	0.00000000	0.00000000	1.77781100	0.00000000	0.00000000	1.87445200
	Sb	-2.23847800	0.00000000	0.11875700	-2.20432700	0.00000000	0.04637700
	C	0.00000000	1.40198400	-2.24522400	0.00000000	1.30308400	-2.16743500
	C	0.00000000	-1.40198400	-2.24522400	0.00000000	-1.30308400	-2.16743500
	O	0.00000000	2.25227100	-3.02698700	0.00000000	2.13045300	-3.00412100
	O	0.00000000	-2.25227100	-3.02698700	0.00000000	-2.13045300	-3.00412100
	Fe	0.00000000	0.00000000	-1.05411900	0.00000000	0.00000000	-1.00970500
2e	Sb	0.00000000	0.00000000	2.97958200	0.00000000	0.00000000	2.94808000
	Sb	1.31647900	-0.00144000	-1.83125300	1.33356900	0.00216500	-1.79653000
	Sb	-1.31647900	0.00144000	-1.83125300	-1.33356900	-0.00216500	-1.79653000
	Fe	0.00000000	0.00000000	0.52848700	0.00000000	0.00000000	0.50437400
	C	0.00000000	1.81242200	0.70820400	0.00000000	1.80173200	0.66605300
	C	0.00000000	-1.81242200	0.70820400	0.00000000	-1.80173200	0.66605300
	O	0.00483900	2.96580000	0.78687600	0.00125000	2.97150400	0.73672900
	O	-0.00483900	-2.96580000	0.78687600	-0.00125000	-2.97150400	0.73672900
2f	Sb	-1.19922000	-1.77526200	0.00000000	-1.13702200	-1.82435300	0.00000000
	Sb	0.00000000	0.66679300	0.00000000	0.00000000	0.68089700	0.00000000
	Sb	-1.01737000	3.14897400	0.00000000	-1.11889700	3.11295900	0.00000000
	Fe	1.39856500	-1.47617300	0.00000000	1.42981900	-1.41606500	0.00000000
	C	3.10561300	-0.96971800	0.00000000	3.11927700	-0.89272700	0.00000000
	C	1.62381600	-3.22452700	0.00000000	1.66847600	-3.15081200	0.00000000
	O	4.23067700	-0.69624000	0.00000000	4.26065400	-0.61393800	0.00000000
	O	1.80767600	-4.36873700	0.00000000	1.88310100	-4.30677600	0.00000000
2g	Sb	0.00000000	0.00000000	0.35942900	0.00000000	0.00000000	0.36367500
	Sb	1.43606700	0.00000000	-2.09459300	1.44920200	0.00000000	-2.07525500
	Sb	-1.43606700	0.00000000	-2.09459300	-1.44920200	0.00000000	-2.07525500
	Fe	0.00000000	0.00000000	2.81066800	0.00000000	0.00000000	2.77996400
	C	0.00000000	1.39784500	3.92581300	0.00000000	1.38909700	3.86544800
	C	0.00000000	-1.39784500	3.92581300	0.00000000	-1.38909700	3.86544800
	O	0.00000000	-2.26518000	4.69565400	0.00000000	-2.26294800	4.65400900
	O	0.00000000	2.26518000	4.69565400	0.00000000	2.26294800	4.65400900
2h	Sb	-2.81031800	0.06503500	0.00000000	-3.00596900	0.04099900	0.00000000
	Sb	1.03406200	-0.15990900	0.00000000	1.05916000	-0.15608600	0.00000000
	Sb	2.65047200	-2.13350400	0.00000000	2.91839900	-1.93299300	0.00000000
	Fe	-0.87630100	1.29727400	0.00000000	-0.97062800	1.12686600	0.00000000
	C	-0.77861500	2.42493900	1.34853100	-0.86838400	2.24612000	1.34572700
	C	-0.77861500	2.42493900	-1.34853100	-0.86838400	2.24612000	-1.34572700
	O	-0.77861500	3.17617800	2.22806900	-0.86838400	3.01250700	2.23388300
	O	-0.77861500	3.17617800	-2.22806900	-0.86838400	3.01250700	-2.23388300
$Sb_2Fe(CO)_3^-$							
3a	Sb	-0.69885200	0.95344900	1.31793600	-0.68551200	0.96063200	1.32742700

	Sb	-0.69885200	0.95344900	-1.31793600	-0.68551200	0.96063200	-1.32742700
	Fe	0.57397300	-0.93868400	0.00000000	0.56017500	-0.92136000	0.00000000
	C	0.52944700	-2.05309000	1.38708400	0.49896900	-2.02468900	1.38163900
	C	0.52944700	-2.05309000	-1.38708400	0.49896900	-2.02468900	-1.38163900
	C	2.33582200	-0.43558200	0.00000000	2.29868800	-0.49526800	0.00000000
	O	0.52944700	-2.80063900	-2.27238600	0.49896900	-2.78826400	-2.27456100
	O	0.52944700	-2.80063900	2.27238600	0.49896900	-2.78826400	2.27456100
	O	3.44002200	-0.09814800	0.00000000	3.44930600	-0.26862400	0.00000000
	Sb	-1.81809900	-0.17299400	0.00000000	1.82961500	-0.10449500	0.00000000
	Sb	0.47473300	-1.70162300	0.00000000	-0.38984200	1.75709000	0.00000000
	Fe	0.50167700	0.98847600	0.00000000	-0.60342200	-0.81858300	0.00000000
	C	0.51617300	1.95928700	1.57686300	-0.54711600	-1.66856800	1.58140500
3b	C	2.27254500	0.51280200	0.00000000	-2.36327800	-0.55378200	0.00000000
	C	0.51617300	1.95928700	-1.57686300	-0.54711600	-1.66856800	-1.58140500
	O	3.42249600	0.38691900	0.00000000	-3.53006700	-0.43889900	0.00000000
	O	0.51617300	2.51384100	2.58389600	-0.54711600	-2.25890300	2.59198400
	O	0.51617300	2.51384100	-2.58389600	-0.54711600	-2.25890300	-2.59198400
	Sb	0.31781600	-1.03483700	1.37622400	0.32370500	-1.00025100	1.39055300
	Sb	0.31781600	-1.03483700	-1.37622400	0.32370500	-1.00025100	-1.39055300
	Fe	-0.29476300	1.17515100	0.00000000	-0.34325100	1.15355300	0.00000000
	C	0.31781600	1.89572700	1.57922500	0.32370500	1.85596100	1.51581500
3c	C	0.31781600	1.89572700	-1.57922500	0.32370500	1.85596100	-1.51581500
	C	-2.15037300	1.01844000	0.00000000	-2.13284300	0.86608600	0.00000000
	O	0.66461000	2.46201200	-2.52466300	0.69542600	2.44179100	-2.46383100
	O	0.66461000	2.46201200	2.52466300	0.69542600	2.44179100	2.46383100
	O	-3.28733400	0.84348900	0.00000000	-3.28844400	0.68706400	0.00000000
	Fe	-1.66842900	0.15693900	0.00049700	0.48597600	1.57897300	0.00000000
	C	-2.79760500	-0.19413000	-1.38804700	0.46039600	2.73962700	1.35328400
	C	-2.77959000	-0.14672500	1.41397200	2.22300700	1.11328700	0.00000000
	C	-1.63024600	1.99729100	-0.02980500	0.46039600	2.73962700	-1.35328400
3d	O	-3.47633500	-0.34570600	2.31389400	3.36622900	0.86681500	0.00000000
	O	-1.61915900	3.14956700	-0.04889700	0.46039600	3.51068600	-2.23624000
	O	-3.50491600	-0.42425200	-2.27213900	0.46039600	3.51068600	2.23624000
	Sb	0.54042100	-1.22430200	0.00148000	-1.28071500	-0.22122500	0.00000000
	Sb	2.50716800	0.57614700	-0.00015700	-0.00937100	-2.59669700	0.00000000
	Fe	-0.80149800	1.79092200	0.00000000	-0.56913200	1.87020700	0.00000000
	C	-0.72740900	2.84209800	1.45262000	-0.47620300	2.86838700	1.46799000
	C	-0.72740900	2.84209800	-1.45262000	-0.47620300	2.86838700	-1.46799000
	C	-2.54960400	1.38240000	0.00000000	-2.30059500	1.58867900	0.00000000
3e	O	-0.72740900	3.55666900	-2.36213100	-0.47620300	3.58356100	-2.39808600
	O	-3.67937100	1.13890900	0.00000000	-3.46345700	1.43701700	0.00000000
	O	-0.72740900	3.55666900	2.36213100	-0.47620300	3.58356100	2.39808600
	Sb	0.36283100	-0.32245200	0.00000000	0.37661100	-0.32099800	0.00000000
	Sb	1.32224800	-2.71640200	0.00000000	0.98892500	-2.84392800	0.00000000
	Fe	0.00000000	0.00000000	0.29153600	0.00000000	0.00000000	0.29346300
	Sb	2.41040700	0.00000000	-0.44025400	2.38712200	0.00000000	-0.41943600
	Sb	-2.41040700	0.00000000	-0.44025400	-2.38712200	0.00000000	-0.41943600
	C	0.00000000	0.00000000	2.04688900	0.00000000	0.00000000	2.03567600
3f	C	0.00000000	1.78762300	0.04732000	0.00000000	1.77270700	-0.00819800
	C	0.00000000	-1.78762300	0.04732000	0.00000000	-1.77270700	-0.00819800
	O	0.00000000	0.00000000	3.20213800	0.00000000	0.00000000	3.20776600
	O	0.00000000	2.93649800	-0.07127100	0.00000000	2.93322300	-0.16408500
	O	0.00000000	-2.93649800	-0.07127100	0.00000000	-2.93322300	-0.16408500

$Sb_3Fe(CO)_3^-$							
4a	Fe	0.00000000	0.00000000	1.25433300	0.00000000	0.00000000	1.25394400
	C	-1.36989500	0.79090900	2.04000500	-1.36266800	0.78673700	2.04215900
	C	0.00000000	-1.58181800	2.04000500	0.00000000	-1.57347300	2.04215900
	C	1.36989500	0.79090900	2.04000500	1.36266800	0.78673700	2.04215900
	O	0.00000000	-2.59732300	2.59185300	0.00000000	-2.59768800	2.61184600
	O	2.24934800	1.29866100	2.59185300	2.24966400	1.29884400	2.61184600
	O	-2.24934800	1.29866100	2.59185300	-2.24966400	1.29884400	2.61184600
	Sb	0.00000000	1.64246700	-0.85972000	0.00000000	1.64514300	-0.86304400
	Sb	-1.42241800	-0.82123300	-0.85972000	-1.42473500	-0.82257100	-0.86304400
	Sb	1.42241800	-0.82123300	-0.85972000	1.42473500	-0.82257100	-0.86304400
4b	Fe	0.08477100	1.58963900	0.00000000	0.08859800	1.56504000	0.00000000
	C	0.50744700	2.65009500	1.36316400	0.51212100	2.60653800	1.36369800
	C	0.50744700	2.65009500	-1.36316400	0.51212100	2.60653800	-1.36369800
	C	-1.74037700	1.75799400	0.00000000	-1.68874500	1.77527400	0.00000000
	O	0.77006600	3.37407300	-2.22675000	0.76828700	3.33982500	-2.24300700
	O	-2.88189300	1.90443600	0.00000000	-2.83542900	2.00292500	0.00000000
	O	0.77006600	3.37407300	2.22675000	0.76828700	3.33982500	2.24300700
	Sb	0.77006600	-0.52509500	1.43600600	0.76828700	-0.52217300	1.44204100
	Sb	0.77006600	-0.52509500	-1.43600600	0.76828700	-0.52217300	-1.44204100
	Sb	-1.28752600	-1.94785600	0.00000000	-1.29982300	-1.93765000	0.00000000
4c	Fe	0.58715300	0.98993500	0.00000000	0.58390400	0.98613200	0.00000000
	C	0.27204500	2.13270200	1.32019900	0.27606700	2.12507400	1.31696900
	C	2.35290700	0.87106200	0.00000000	2.34219600	0.87130800	0.00000000
	C	0.27204500	2.13270200	-1.32019900	0.27606700	2.12507400	-1.31696900
	O	3.50719000	0.84329700	0.00000000	3.51267000	0.85540300	0.00000000
	O	0.08922800	2.92254100	-2.14214500	0.09809900	2.93264300	-2.14537100
	O	0.08922800	2.92254100	2.14214500	0.09809900	2.93264300	2.14537100
	Sb	-1.76238600	-0.38053500	0.00000000	-1.77210200	-0.38610900	0.00000000
	Sb	0.27204500	-0.88879300	1.87648300	0.27606700	-0.88668700	1.87135900
	Sb	0.27204500	-0.88879300	-1.87648300	0.27606700	-0.88668700	-1.87135900
4d	Fe	0.05142700	1.67457800	0.00000000	0.05362600	1.68350400	0.00000000
	C	0.50528500	2.78112300	1.31051900	0.50828100	2.78496100	1.30807100
	C	0.50528500	2.78112300	-1.31051900	0.50828100	2.78496100	-1.30807100
	C	-1.71258900	1.61892800	0.00000000	-1.71027700	1.64023800	0.00000000
	O	0.76009100	3.52725300	-2.15803300	0.76204500	3.54349600	-2.16666700
	O	-2.86869400	1.65831300	0.00000000	-2.88127700	1.68997100	0.00000000
	O	0.76009100	3.52725300	2.15803300	0.76204500	3.54349600	2.16666700
	Sb	0.50528500	-0.33800500	1.49451600	0.50828100	-0.33738000	1.48991600
	Sb	0.50528500	-0.33800500	-1.49451600	0.50828100	-0.33738000	-1.48991600
	Sb	-0.74266700	-2.38925700	0.00000000	-0.74939500	-2.40853000	0.00000000
4e	Fe	0.00000000	0.00000000	-1.41471200	0.00000000	0.00000000	-1.35057400
	Sb	-2.06561800	0.00000000	0.21960900	-2.08446800	0.00000000	0.19490400
	Sb	2.06561800	0.00000000	0.21960900	2.08446800	0.00000000	0.19490400
	Sb	0.00000000	0.00000000	2.09672100	0.00000000	0.00000000	2.05722100
	C	0.00000000	1.80837400	-1.34679800	0.00000000	1.79869600	-1.28518300
	C	0.00000000	-1.80837400	-1.34679800	0.00000000	-1.79869600	-1.28518300
	C	0.00000000	0.00000000	-3.22080300	0.00000000	0.00000000	-3.12287200
	O	0.00000000	2.96223400	-1.37782800	0.00000000	2.96848200	-1.32163800
	O	0.00000000	-2.96223400	-1.37782800	0.00000000	-2.96848200	-1.32163800
	O	0.00000000	0.00000000	-4.37734400	0.00000000	0.00000000	-4.29724600
4f	Fe	0.56431900	0.99624800	0.00000000	0.56185600	1.00418300	0.00000000
	C	0.36522500	2.09362900	1.37538000	0.35844200	2.11375700	1.35696100

	C	2.34626200	0.85096400	0.00000000	2.33741600	0.85433800	0.00000000
	C	0.36522500	2.09362900	-1.37538000	0.35844200	2.11375700	-1.35696100
	O	3.49794300	0.80014500	0.00000000	3.50524700	0.80487600	0.00000000
	O	0.26613500	2.83964800	-2.25041900	0.26012000	2.88509800	-2.23078000
	O	0.26613500	2.83964800	2.25041900	0.26012000	2.88509800	2.23078000
	Sb	-2.01229800	0.61928000	0.00000000	-1.99410000	0.56229000	0.00000000
	Sb	0.36522500	-1.36814300	1.33737000	0.35844200	-1.35173700	1.34932400
	Sb	0.36522500	-1.36814300	-1.33737000	0.35844200	-1.35173700	-1.34932400
	Fe	1.77651000	0.00594600	-0.00119100	1.73324100	-0.00213300	-0.00163600
	C	2.89647900	1.41103800	-0.00327200	2.85885400	1.36234800	-0.00338100
	C	2.43934400	-0.84023000	1.44221700	2.36455700	-0.80748000	1.44537400
	C	2.44055400	-0.84965000	-1.43877800	2.36678400	-0.81849300	-1.44196500
4g	O	2.91023700	-1.37397600	2.35177900	2.85245000	-1.32692900	2.37609500
	O	2.91119600	-1.39598700	-2.34095600	2.85635500	-1.35507800	-2.36200300
	O	3.63959200	2.29527900	-0.00261400	3.63193600	2.24355700	-0.00216100
	Sb	-0.38962100	-1.55273100	0.00129000	-0.34359100	-1.55898400	0.00162600
	Sb	-0.23637600	1.55045100	-0.00262000	-0.23637000	1.56733900	-0.00336200
	Sb	-2.67862500	0.10651300	0.00062900	-2.66183100	0.09252400	0.00069600
	Fe	-1.76102800	0.69749600	-0.00765700	1.77538300	0.59558000	-0.00146100
	C	-2.68852100	0.52758500	1.52830800	2.72870000	0.21295100	-1.44165500
	C	-1.73660200	2.47015300	-0.15445800	2.01806600	2.34708100	0.00219100
	C	-2.93203400	0.33440200	-1.30941300	2.70076600	0.21603900	1.45683200
4h	O	-1.75669500	3.61917300	-0.25379900	2.22157600	3.49951700	0.00360400
	O	-3.72739400	0.11450900	-2.11685100	3.39145200	-0.00992400	2.37601500
	O	-3.32402100	0.40586100	2.48268600	3.43871400	-0.02025600	-2.34411500
	Sb	-0.99349600	-1.85794300	-0.01555100	0.84467600	-1.86191900	0.00086000
	Sb	0.73781400	0.27211600	0.00597000	-0.71538800	0.54519800	-0.01017000
	Sb	3.40067300	0.18888400	-0.01167100	-3.33044700	0.14228600	0.00244200
	Fe	2.36250800	0.65885700	0.00000000	2.38823600	0.64495300	0.00000000
	C	2.30854700	-0.11704700	1.57689900	2.31973300	-0.19127900	1.53945000
	C	2.30854700	-0.11704700	-1.57689900	2.31973300	-0.19127900	-1.53945000
	C	4.08680800	1.04846700	0.00000000	4.09521700	1.11049700	0.00000000
4i	O	2.30854700	-0.78518700	-2.52813000	2.31973300	-0.89696500	-2.48283700
	O	5.20591900	1.34792600	0.00000000	5.22232400	1.44120400	0.00000000
	O	2.30854700	-0.78518700	2.52813000	2.31973300	-0.89696500	2.48283700
	Sb	-0.10625500	1.18024800	0.00000000	-0.04118600	1.11791000	0.00000000
	Sb	-1.83150700	-0.78852600	1.35236400	-1.87545100	-0.73851000	1.36700700
	Sb	-1.83150700	-0.78852600	-1.35236400	-1.87545100	-0.73851000	-1.36700700
	Fe	1.63382200	0.74272300	-0.00004700	1.60944200	0.75987300	0.00682800
	C	1.52745800	1.91833700	-1.32760500	1.50262900	1.96686100	-1.28055500
	C	1.51670000	1.91188200	1.33221900	1.57988600	1.90560000	1.34686600
	C	3.37219600	0.33969000	0.00130800	3.32586700	0.31549500	-0.09897400
4j	O	1.47270000	2.64876300	2.21477400	1.61652800	2.65524700	2.24213800
	O	4.51289000	0.16220500	0.00099900	4.47768600	0.11697000	-0.16532300
	O	1.49369300	2.66170900	-2.20514700	1.47038300	2.75745100	-2.13887100
	Sb	1.39724400	-1.79044300	-0.00027400	1.38234200	-1.77442200	0.32465300
	Sb	-0.78061400	-0.02925200	-0.00072700	-0.80313900	-0.01806600	0.04558200
	Sb	-3.37764500	0.09201500	-0.00133900	-3.39318000	-0.02738000	-0.26818300
	Fe	1.02694100	0.09761100	0.47357300	1.04695500	0.17307200	0.50023100
	Sb	3.20418900	-0.52831000	-0.47896000	3.15375500	-0.62811200	-0.50064100
4k	Sb	-1.17016400	0.90273800	-0.64358600	-1.15684200	0.84737700	-0.62451300
	Sb	-3.31817000	-0.50250900	-0.02606800	-3.34700400	-0.51329500	-0.05760800
	C	0.64332500	-1.64446400	0.22184700	0.65778400	-1.57916800	0.50991000

	C	0.48843600	0.17300000	2.15109400	0.56511400	0.49014200	2.16203800
	C	1.71421100	1.76468000	0.37248900	1.78828800	1.77359400	0.13584600
	O	0.37978900	-2.76003900	0.10247200	0.38242400	-2.71284200	0.56837800
	O	0.21105600	0.19579000	3.26970100	0.32725200	0.67344200	3.29215000
	O	2.12354400	2.84361800	0.35205600	2.23616200	2.83792900	-0.05201700
	Fe	2.86821300	-0.77661000	0.00000000	2.88268800	-0.65626800	0.00000000
	C	2.82622900	-1.81659500	1.44679900	2.82090000	-1.65674100	1.44542900
	C	2.82622900	-1.81659500	-1.44679900	2.82090000	-1.65674100	-1.44542900
	C	4.59418700	-0.29123800	0.00000000	4.60827800	-0.22764700	0.00000000
4l	O	2.82622900	-2.55174100	-2.33627800	2.82090000	-2.41448000	-2.33930100
	O	5.70375600	0.02527000	0.00000000	5.74477400	0.05530100	0.00000000
	O	2.82622900	-2.55174100	2.33627800	2.82090000	-2.41448000	2.33930100
	Sb	0.69649100	0.19592000	0.00000000	0.70378800	0.27697700	0.00000000
	Sb	-1.95865100	-0.52119100	0.00000000	-1.90948400	-0.61260500	0.00000000
	Sb	-3.18692100	1.97946900	0.00000000	-3.25593100	1.83560800	0.00000000

Table S4 The Cartesian coordinates (Å) of the structures of $Bi_mFe(CO)_n^-$ (m, n = 2, 3) optimized at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O), and BP86/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) levels, respectively.

Isomer		B3LYP			BP86		
$Bi_2Fe(CO)_2^-$							
1a′	Fe	0.00000000	0.00000000	1.51883700	0.00000000	0.00000000	1.50146900
	C	0.00000000	1.39247000	2.61057200	0.00000000	1.38188300	2.59291500
	C	0.00000000	-1.39247000	2.61057200	0.00000000	-1.38188300	2.59291500
	O	0.00000000	2.28062900	3.36321400	0.00000000	2.27016000	3.36992200
	O	0.00000000	-2.28062900	3.36321400	0.00000000	-2.27016000	3.36992200
	Bi	0.00000000	1.39950000	-0.75077100	0.00000000	1.40648800	-0.74742100
	Bi	0.00000000	-1.39950000	-0.75077100	0.00000000	-1.40648800	-0.74742100
1b′	Fe	0.00000000	0.00000000	1.62603400	0.00000000	0.00000000	1.54178600
	C	0.00000000	1.68149600	2.36069100	0.00000000	1.55815400	2.42142900
	C	0.00000000	-1.68149600	2.36069100	0.00000000	-1.55815400	2.42142900
	O	0.00000000	2.73171200	2.84736600	0.00000000	2.57197900	3.01731100
	O	0.00000000	-2.73171200	2.84736600	0.00000000	-2.57197900	3.01731100
	Bi	0.00000000	1.43891000	-0.69977700	0.00000000	1.46618500	-0.70735300
	Bi	0.00000000	-1.43891000	-0.69977700	0.00000000	-1.46618500	-0.70735300
1c′	Fe	0.00000000	0.00000000	1.55796300	0.00000000	0.00000000	1.51755600
	C	0.00000000	1.53004700	2.61771100	0.00000000	1.45246300	2.59934000
	C	0.00000000	-1.53004700	2.61771100	0.00000000	-1.45246300	2.59934000
	O	0.00000000	2.51338600	3.22864600	0.00000000	2.37327000	3.33243800
	O	0.00000000	-2.51338600	3.22864600	0.00000000	-2.37327000	3.33243800
	Bi	-1.40437800	0.00000000	-0.74444500	-1.41293500	0.00000000	-0.74679200
	Bi	1.40437800	0.00000000	-0.74444500	1.41293500	0.00000000	-0.74679200
1d′	Fe	0.00000000	0.00000000	-2.77250200	0.00000000	0.00000000	-2.73737400
	Bi	0.00000000	0.00000000	-0.20271700	0.00000000	0.00000000	-0.23231900
	Bi	0.00000000	0.00000000	2.51696700	0.00000000	0.00000000	2.49525500
	C	0.00000000	1.43480800	-3.85579500	0.00000000	1.46111200	-3.73975200
	C	0.00000000	-1.43480800	-3.85579500	0.00000000	-1.46111200	-3.73975200
	O	0.00000000	-2.32110800	-4.60800600	0.00000000	-2.37530900	-4.48593200
	O	0.00000000	2.32110800	-4.60800600	0.00000000	2.37530900	-4.48593200
$Bi_3Fe(CO)_2^-$							
2a′	Bi	1.54206500	-0.94508300	-0.00002300	1.62370400	-0.79685600	-0.00002900
	Bi	-0.99568800	-0.28412800	-1.47953800	-0.95513000	-0.37008300	-1.48906300
	Bi	-0.99562200	-0.28409000	1.47958700	-0.95506100	-0.37004200	1.48911700
	Fe	0.52370000	1.53576100	-0.00003100	0.33855300	1.56205500	-0.00002700
	C	2.11136600	2.35994900	-0.00007000	1.84399900	2.50429800	-0.00006600
	C	-0.59289700	2.90159500	-0.00002000	-0.88022200	2.81901700	-0.00002100
	O	-1.29748500	3.82652800	-0.00002000	-1.66209200	3.70292200	-0.00002500
	O	3.11752100	2.93658300	-0.00008600	2.81127000	3.17409900	-0.00008200
2b′	Bi	-1.64636000	0.35591100	0.00000000	-1.64839100	0.33094300	0.00000000
	Bi	0.61058300	-0.89459300	1.49334500	0.61272200	-0.88849200	1.49989900
	Bi	0.61058300	-0.89459300	-1.49334500	0.61272200	-0.88849200	-1.49989900
	Fe	0.79369700	1.41248700	0.00000000	0.78391500	1.41763100	0.00000000
	C	0.61058300	2.50306300	-1.35756200	0.61272200	2.51987400	-1.33580500
	C	0.61058300	2.50306300	1.35756200	0.61272200	2.51987400	1.33580500

	O	0.45800000	3.26251900	-2.22423000	0.46063100	3.30778100	-2.20225900
	O	0.45800000	3.26251900	2.22423000	0.46063100	3.30778100	2.20225900
2c′	Bi	0.10219600	-1.51073600	0.75785600	-0.00361800	-1.55321100	0.65609300
	Bi	1.99372500	0.16224400	-0.75443000	2.03460100	0.14760500	-0.74961600
	Bi	-2.04765300	-0.06336400	-0.51982300	-2.10128200	0.08828300	-0.47372500
	Fe	-0.05832200	1.42029700	0.41846500	0.05032100	1.27303400	0.50215400
	C	1.15115600	2.23024500	1.42570000	1.24484500	1.90789800	1.61461700
	C	-1.31969300	2.67624100	0.45537900	-0.99974800	2.69460000	0.40643900
	O	1.88735600	2.79202000	2.12597500	1.98412600	2.37553600	2.40404200
	O	-2.07219200	3.56014900	0.46081900	-1.60213800	3.70245600	0.33336200
2d′	Bi	2.32583100	0.00000000	-0.11871800	2.28351200	0.00000000	-0.19291700
	Bi	0.00000000	0.00000000	1.63895100	0.00000000	0.00000000	1.74437900
	Bi	-2.32583100	0.00000000	-0.11871800	-2.28351200	0.00000000	-0.19291700
	C	0.00000000	1.39782500	-2.49556500	0.00000000	1.29447600	-2.39627300
	C	0.00000000	-1.39782500	-2.49556500	0.00000000	-1.29447600	-2.39627300
	O	0.00000000	2.23841300	-3.28903500	0.00000000	2.11541100	-3.24125700
	O	0.00000000	-2.23841300	-3.28903500	0.00000000	-2.11541100	-3.24125700
	Fe	0.00000000	0.00000000	-1.29824500	0.00000000	0.00000000	-1.23630600
2e′	Bi	0.00000000	0.00000000	3.13518500	0.00000000	0.00000000	3.09235200
	Bi	1.38271900	0.00000000	-1.79899800	1.39826600	0.00000000	-1.76437300
	Bi	-1.38271900	0.00000000	-1.79899800	-1.39826600	0.00000000	-1.76437300
	Fe	0.00000000	0.00000000	0.61488100	0.00000000	0.00000000	0.58327100
	C	0.00000000	1.81133900	0.76976700	0.00000000	1.80022200	0.72240600
	C	0.00000000	-1.81133900	0.76976700	0.00000000	-1.80022200	0.72240600
	O	0.00000000	2.96743300	0.82432400	0.00000000	2.97278800	0.77417700
	O	0.00000000	-2.96743300	0.82432400	0.00000000	-2.97278800	0.77417700
2f′	Bi	3.07969100	0.38995700	0.00000000	3.28216700	0.29414800	0.00000000
	Bi	-0.96746000	0.04389800	0.00000000	-0.96765100	0.03420800	0.00000000
	Bi	-2.74796200	-1.97188200	0.00000000	-3.03012300	-1.72193700	0.00000000
	Fe	1.02267300	1.55270200	0.00000000	1.14880800	1.33445200	0.00000000
	C	0.93486400	2.67936700	1.34323800	1.05451400	2.44975700	1.34445100
	C	0.93486400	2.67936700	-1.34323800	1.05451400	2.44975700	-1.34445100
	O	0.93486400	3.44584800	2.21121100	1.05451400	3.22340100	2.22797000
	O	0.93486400	3.44584800	-2.21121100	1.05451400	3.22340100	-2.22797000
$Bi_2Fe(CO)_3^-$							
3a′	Bi	-0.50626800	0.71299500	1.38410500	-0.82876100	0.48468700	1.36988400
	Bi	-0.50626800	0.71299500	-1.38410500	-0.26223700	1.12227700	-1.31083300
	Fe	0.76739600	-1.24596100	0.00000000	0.72245300	-1.10098800	-0.04019300
	C	0.70504100	-2.35052000	1.39141200	0.64889500	-2.24981600	1.29620900
	C	0.70504100	-2.35052000	-1.39141200	0.58572100	-2.11438000	-1.48722600
	C	2.53324200	-0.76670000	0.00000000	2.46282800	-0.75129300	-0.12819500
	O	0.70504100	-3.09907100	-2.27748100	0.53342600	-2.81014800	-2.43274200
	O	0.70504100	-3.09907100	2.27748100	0.66156600	-3.05650500	2.15153200
	O	3.64344200	-0.44631700	0.00000000	3.61897700	-0.55757600	-0.19114600
3b′	Bi	-1.68925200	0.19823500	0.00000000	1.68160900	-0.39684700	0.00000000
	Bi	0.64478900	-1.52389100	0.00000000	-0.61121800	1.60413500	0.00000000
	Fe	0.77359700	1.22851700	0.00000000	-0.83659700	-1.03747400	0.00000000
	C	0.79108000	2.18911600	1.58101100	-0.77021000	-1.92687200	1.55265400
	C	2.51775600	0.66338200	0.00000000	-2.58526100	-0.73287500	0.00000000
	C	0.79108000	2.18911600	-1.58101100	-0.77021000	-1.92687200	-1.55265400
	O	3.66501400	0.49955600	0.00000000	-3.75168100	-0.59707200	0.00000000
	O	0.79108000	2.74011700	2.59121800	-0.77021000	-2.55839000	2.54019100

	O	0.79108000	2.74011700	-2.59121800	-0.77021000	-2.55839000	-2.54019100
	Bi	0.23306700	-0.76873100	1.44253400	0.23719100	-0.73810800	1.45657200
	Bi	0.23306700	-0.76873100	-1.44253400	0.23719100	-0.73810800	-1.45657200
	Fe	-0.38606500	1.49897300	0.00000000	-0.44558500	1.46293500	0.00000000
	C	0.23306700	2.18125000	1.59123800	0.23719100	2.15463000	1.51029200
3c′	C	0.23306700	2.18125000	-1.59123800	0.23719100	2.15463000	-1.51029200
	C	-2.23779400	1.39085700	0.00000000	-2.22858600	1.15117200	0.00000000
	O	0.56522900	2.74815100	-2.54411800	0.61351600	2.74941600	-2.45316900
	O	0.56522900	2.74815100	2.54411800	0.61351600	2.74941600	2.45316900
	O	-3.38314700	1.26818200	0.00000000	-3.38494300	0.96704200	0.00000000
	Bi	-0.01713200	-1.20534300	-0.00007600	0.03250800	-1.17358400	0.00691400
	Bi	-2.20629300	0.57257000	0.00039800	-2.23990900	0.54246300	0.00049800
	Fe	2.13021700	0.39750600	-0.00012800	2.10409600	0.36923000	0.00846800
	C	3.67542400	-0.47327300	-0.45797400	3.67189800	-0.47521300	-0.19247300
3d′	C	2.18380500	1.84231500	-1.12142100	2.22921400	1.60326300	-1.27330300
	C	2.61951200	1.16857100	1.57538400	2.46796400	1.37919100	1.43060800
	O	2.21827700	2.75226600	-1.83081600	2.34176900	2.41692800	-2.10883900
	O	4.64179100	-1.03781800	-0.74666500	4.71358300	-0.99714500	-0.32593900
	O	2.92571200	1.65547000	2.57756400	2.73131700	2.04766400	2.35673000
	Bi	0.04280500	0.08540600	0.00000000	0.10225600	0.12803200	0.00000000
	Bi	1.44016700	-2.25783800	0.00000000	1.13747700	-2.41238700	0.00000000
	Fe	-1.34579700	2.16932200	0.00000000	-1.05719000	2.29094800	0.00000000
	C	-3.08762200	1.70937400	0.00000000	-2.78304200	1.97388400	0.00000000
3e′	C	-1.28218800	3.23716400	1.44502600	-0.97055000	3.29487400	1.46065800
	C	-1.28218800	3.23716400	-1.44502600	-0.97055000	3.29487400	-1.46065800
	O	-1.28218800	3.96145200	2.34691700	-0.97055000	4.02036200	2.38370400
	O	-4.20862200	1.42800700	0.00000000	-3.94215700	1.79115800	0.00000000
	O	-1.28218800	3.96145200	-2.34691700	-0.97055000	4.02036200	-2.38370400
$Bi_3Fe(CO)_3^-$							
	Fe	0.00000000	0.00000000	1.55992800	0.00000000	0.00000000	1.55825400
	C	-1.37179700	0.79200700	2.33695300	-1.36601000	0.78866600	2.33637000
	C	0.00000000	-1.58401500	2.33695300	0.00000000	-1.57733200	2.33637000
	C	1.37179700	0.79200700	2.33695300	1.36601000	0.78866600	2.33637000
4a′	O	0.00000000	-2.59892700	2.89338700	0.00000000	-2.60303500	2.90683900
	O	2.25073700	1.29946300	2.89338700	2.25429400	1.30151700	2.90683900
	O	-2.25073700	1.29946300	2.89338700	-2.25429400	1.30151700	2.90683900
	Bi	0.00000000	1.70896600	-0.61070100	0.00000000	1.71104500	-0.61178100
	Bi	-1.48000800	-0.85448300	-0.61070100	-1.48180900	-0.85552300	-0.61178100
	Bi	1.48000800	-0.85448300	-0.61070100	1.48180900	-0.85552300	-0.61178100
	Fe	-1.87686800	0.01083800	0.58772800	-1.84504700	0.00645900	0.58221700
	C	-2.94147500	1.42916200	0.60583100	-2.91133200	1.41282800	0.55181100
	C	-3.05703000	-1.30733600	0.40271700	-2.98779000	-1.33128900	0.42626500
	C	-1.47188700	-0.14867000	2.36586000	-1.50345600	-0.08790800	2.33438400
4b′	O	-3.85461900	-2.14253800	0.30936600	-3.78357100	-2.19363500	0.36364000
	O	-1.24953300	-0.25419300	3.49143800	-1.36183400	-0.15161800	3.49465200
	O	-3.67321800	2.32700900	0.64675900	-3.66148000	2.31718900	0.57353700
	Bi	-0.03382200	1.50021800	-0.78046300	-0.04424500	1.50026400	-0.78455400
	Bi	-0.06085600	-1.47736000	-0.80340900	-0.06056500	-1.48852400	-0.79472000
	Bi	2.06865300	-0.01759200	0.72715100	2.06675900	-0.01059900	0.73027400
	Fe	0.72892800	1.23811300	0.00000000	0.72781900	1.23089500	0.00000000
4c′	C	0.42248900	2.37449500	1.32280500	0.42601400	2.36281500	1.32042700
	C	2.49004300	1.10217100	0.00000000	2.48239000	1.09755600	0.00000000
	C	0.42248900	2.37449500	-1.32280500	0.42601400	2.36281500	-1.32042700

	O	3.64631900	1.07702600	0.00000000	3.65459700	1.07885600	0.00000000
	O	0.25632900	3.17080000	-2.14415700	0.26291800	3.17426800	-2.15046900
	O	0.25632900	3.17080000	2.14415700	0.26291800	3.17426800	2.15046900
	Bi	-1.71526800	-0.14125900	0.00000000	-1.72399500	-0.14039900	0.00000000
	Bi	0.42248900	-0.69230400	1.93577500	0.42601400	-0.69101500	1.92747500
	Bi	0.42248900	-0.69230400	-1.93577500	0.42601400	-0.69101500	-1.92747500
	Fe	0.04685100	2.06889400	0.00000000	0.04523300	2.07741500	0.00000000
	C	0.50345500	3.15573500	1.32069900	0.50287000	3.15588000	1.32275200
	C	0.50345500	3.15573500	-1.32069900	0.50287000	3.15588000	-1.32275200
	C	-1.71596400	2.01413300	0.00000000	-1.71783700	2.04805900	0.00000000
4d′	O	0.75272500	3.88994100	-2.18313300	0.75549300	3.90310400	-2.19424500
	O	-2.87338400	2.06438900	0.00000000	-2.88962600	2.11408600	0.00000000
	O	0.75272500	3.88994100	2.18313300	0.75549300	3.90310400	2.19424500
	Bi	0.50345500	-0.02500000	1.53984300	0.50287000	-0.02004500	1.53449300
	Bi	0.50345500	-0.02500000	-1.53984300	0.50287000	-0.02004500	-1.53449300
	Bi	-0.83848000	-2.14878300	0.00000000	-0.83555200	-2.17116400	0.00000000
	Fe	-0.86105200	1.49664400	0.00000000	-0.71406000	1.47884200	0.00000000
	Bi	-1.89241300	-1.01394900	0.00000000	-1.98322200	-0.86687100	0.00000000
	Bi	1.82692400	1.11446900	0.00000000	1.91099600	1.00698300	0.00000000
	Bi	0.95475800	-1.67432800	0.00000000	0.81866200	-1.70428300	0.00000000
4e′	C	-0.80840600	1.43193900	1.80476800	-0.66497700	1.40622400	1.79581100
	C	-0.80840600	1.43193900	-1.80476800	-0.66497700	1.40622400	-1.79581100
	C	-1.73720200	3.07185100	0.00000000	-1.47987500	3.07523100	0.00000000
	O	-0.80840600	1.46323200	2.96041600	-0.66497700	1.43518400	2.96786300
	O	-0.80840600	1.46323200	-2.96041600	-0.66497700	1.43518400	-2.96786300
	O	-2.29542200	4.08589100	0.00000000	-1.98625700	4.13590900	0.00000000
	Fe	0.71510500	1.26536800	0.00000000	0.71307000	1.26427400	0.00000000
	C	0.50053000	2.36567700	1.36761200	0.49724600	2.36965100	1.35534700
	C	2.49172900	1.11013500	0.00000000	2.48339400	1.10416100	0.00000000
	C	0.50053000	2.36567700	-1.36761200	0.49724600	2.36965100	-1.35534700
4f′	O	3.64515200	1.06635400	0.00000000	3.65298100	1.06120200	0.00000000
	O	0.39761400	3.12095700	-2.23576900	0.39570000	3.14444700	-2.22751500
	O	0.39761400	3.12095700	2.23576900	0.39570000	3.14444700	2.22751500
	Bi	-1.90554900	0.78228800	0.00000000	-1.89765200	0.75781900	0.00000000
	Bi	0.50053000	-1.15267800	1.40825200	0.49724600	-1.14236000	1.41538100
	Bi	0.50053000	-1.15267800	-1.40825200	0.49724600	-1.14236000	-1.41538100
	Fe	2.21203600	0.00774300	-0.00274500	2.18009100	-0.00242600	-0.00014500
	C	3.23471800	1.46693000	-0.02122200	3.19830400	1.44121600	-0.00936200
	C	2.89854700	-0.78463100	1.43095700	2.86237300	-0.78721000	1.43200700
	C	2.91577700	-0.84680700	-1.39401300	2.87340700	-0.81360900	-1.41278000
4g′	O	3.41530200	-1.28602100	2.33753100	3.39521400	-1.29691800	2.34543900
	O	3.44278000	-1.40272700	-2.26196300	3.41394700	-1.34172300	-2.31111500
	O	3.93163000	2.39162800	-0.02943300	3.91206800	2.37386600	-0.01648700
	Bi	-0.01193400	-1.58915700	0.00004200	0.02358700	-1.58407600	-0.00062800
	Bi	0.08965400	1.55372400	-0.00728800	0.07880200	1.57498600	-0.00226200
	Bi	-2.46476700	0.07353700	0.00252300	-2.46451800	0.04690800	0.00050200
	Fe	-1.84261000	1.35806300	0.00000000	-1.75931700	1.43528100	0.00000000
	C	-1.76675900	2.52403300	1.33618300	-1.67854700	2.61288100	1.30753100
	C	-1.76675900	2.52403300	-1.33618300	-1.67854700	2.61288100	-1.30753100
4h′	C	-3.55970600	0.92643200	0.00000000	-3.48559000	1.02205400	0.00000000
	O	-1.76675900	3.27176500	-2.21175700	-1.67854700	3.39388100	-2.17721900
	O	-4.72186700	0.90021000	0.00000000	-4.66322900	1.06998100	0.00000000
	O	-1.76675900	3.27176500	2.21175700	-1.67854700	3.39388100	2.17721900

Bi	-1.91744600	-1.20310700	0.00000000	-1.97175600	-1.12454100	0.00000000
Bi	0.68945700	0.45631800	0.00000000	0.73962200	0.47564700	0.00000000
Bi	3.11365400	-0.82798900	0.00000000	3.05094100	-1.00973500	0.00000000

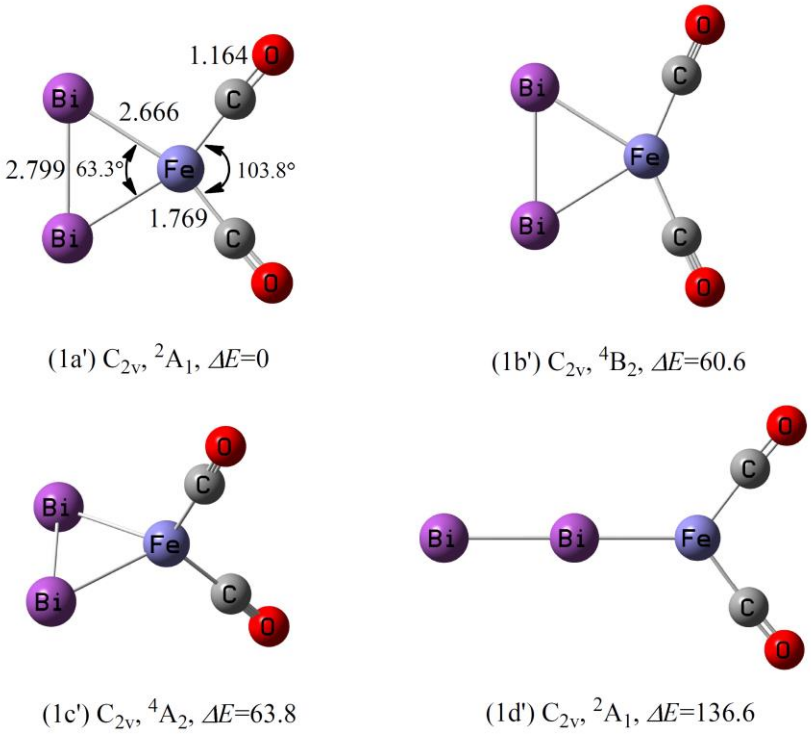

Fig. S1 Optimized structures of the $Bi_2Fe(CO)_2^-$ isomers calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level, including the symmetry, electronic state, and the relative energy with ZPE correction of each isomer (ΔE in kJ/mol).

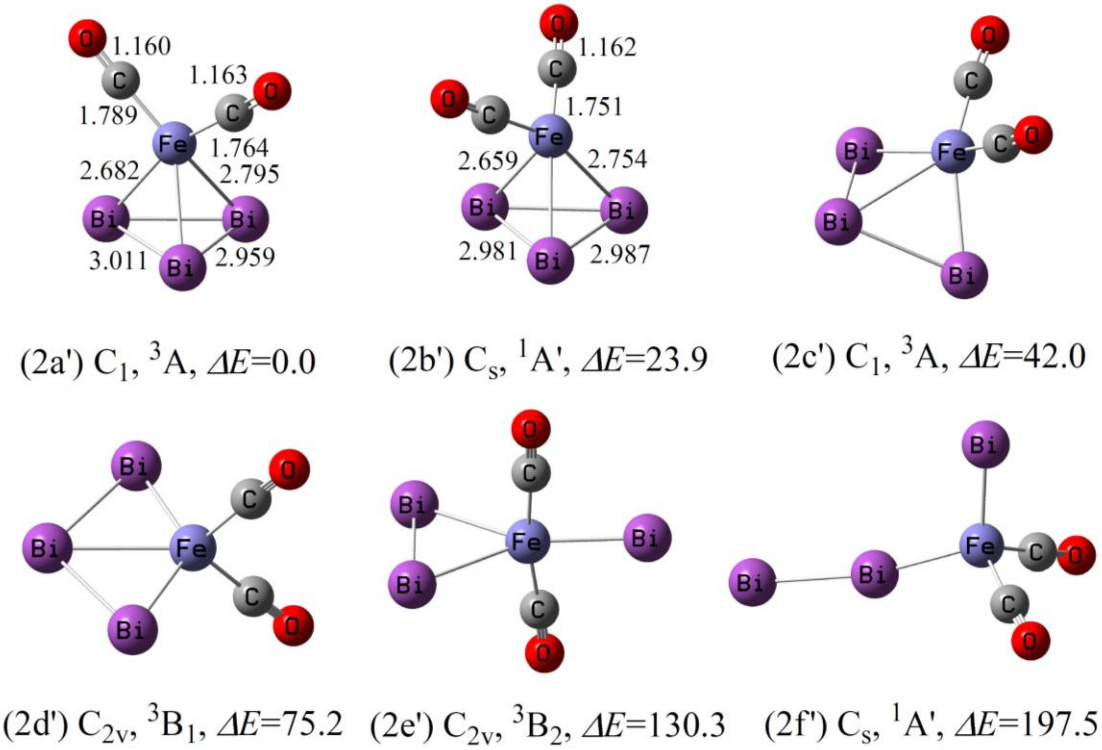

Fig. S2 Optimized structures of the $Bi_3Fe(CO)_2^-$ isomers calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level, including the symmetry, electronic state, and the relative energy with ZPE correction of each isomer (ΔE in kJ/mol).

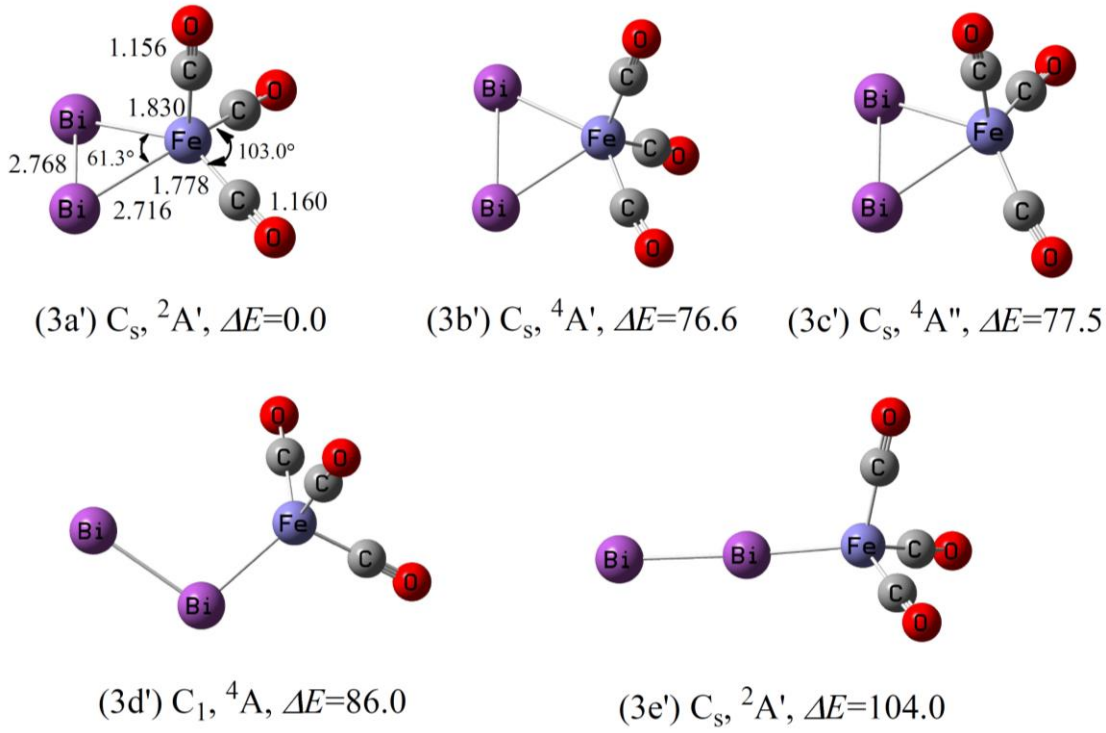

Fig. S3 Optimized structures of the $Bi_2Fe(CO)_3^-$ isomers calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level, including the symmetry, electronic state, and the relative energy with ZPE correction of each isomer (ΔE in kJ/mol).

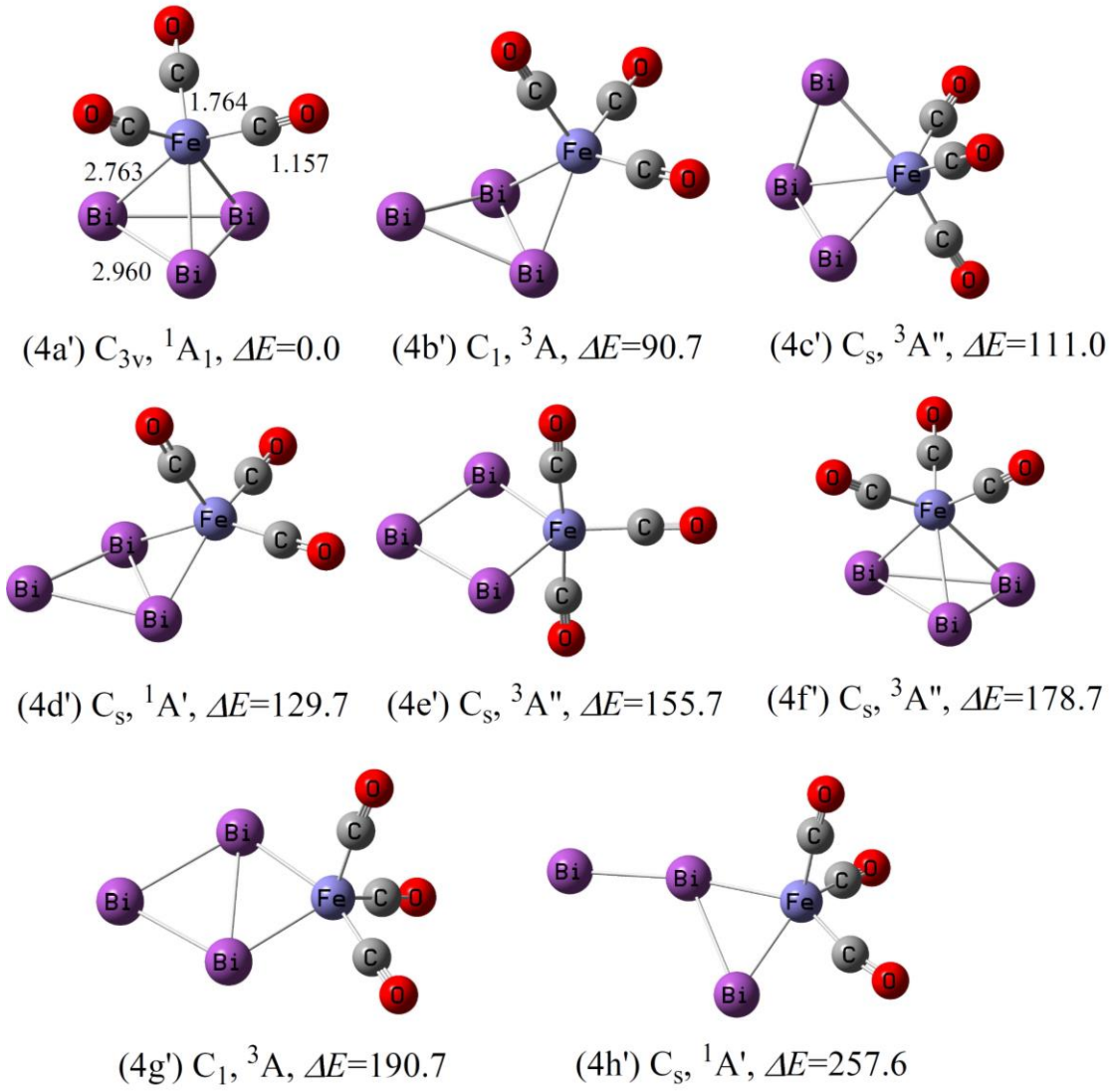

Fig. S4 Optimized structures of the $Bi_3Fe(CO)_3^-$ isomers calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level, including the symmetry, electronic state, and the relative energy with ZPE correction of each isomer (ΔE in kJ/mol).

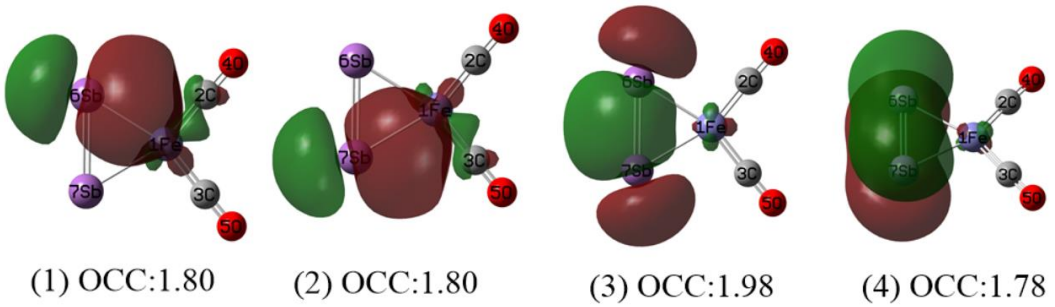

Fig. S5 Natural bonding orbitals related to the Fe−Sb bonds (1, 2) and Sb−Sb bonds (3, 4) in the $Sb_2Fe(CO)_2^-$ (C_{2v}, $^2A_1$) anion calculated at the B3LYP/SDD(Sb)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

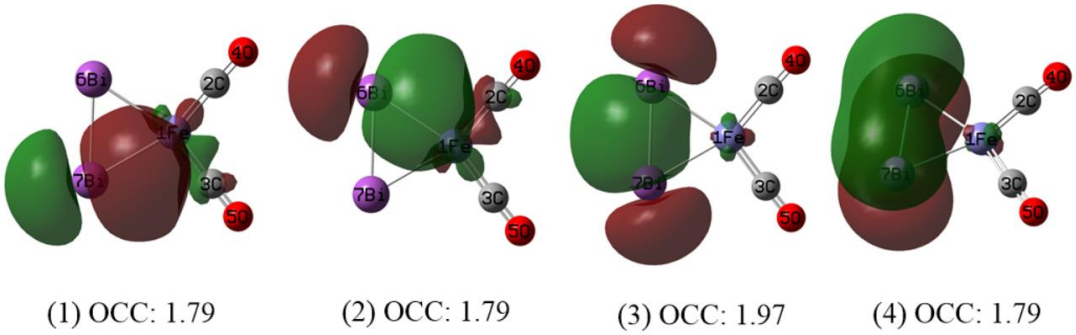

Fig. S6 Natural bonding orbitals related to the Fe−Bi bonds (1, 2) and Bi−Bi bonds (3, 4) in the $Bi_2Fe(CO)_2^-$ (C_{2v}, $^2A_1$) anion calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

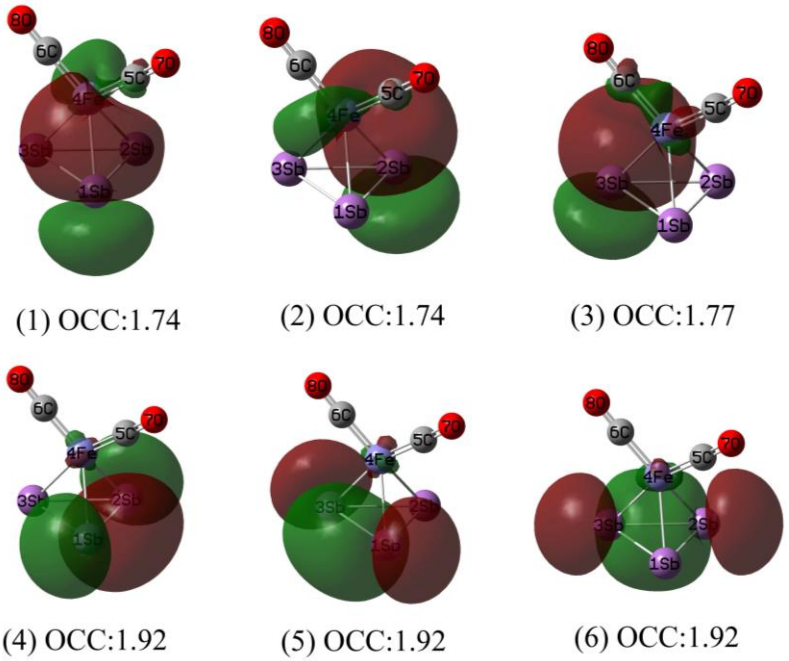

Fig. S7 Natural bonding orbitals related to the Fe−Sb bonds (1−3) and Sb−Sb bonds (4−6) in the $Sb_3Fe(CO)_2^-$ (C_s, ^3A") anion calculated at the B3LYP/SDD(Sb)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

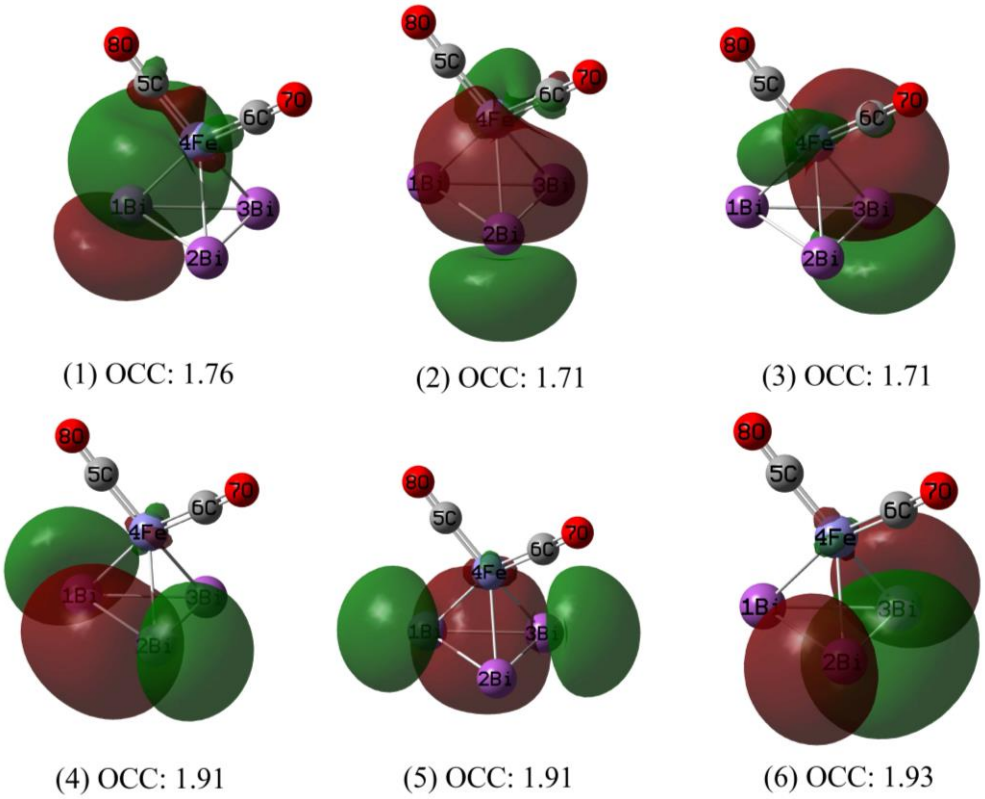

Fig. S8 Natural bonding orbitals related to the Fe−Bi bonds (1−3) and Bi−Bi bonds (4−6) in the $Bi_3Fe(CO)_2^-$ (C_1, ^3A) anion calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

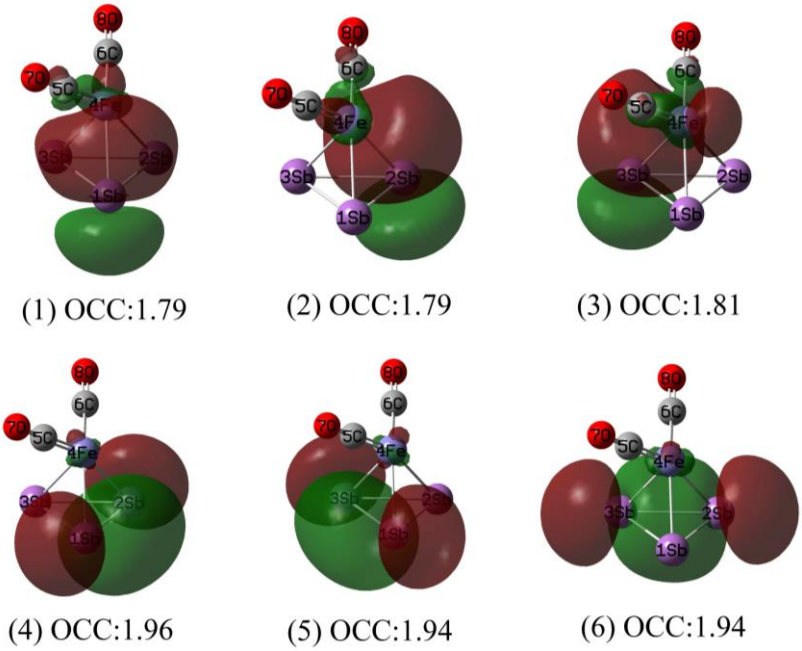

Fig. S9 Natural bonding orbitals related to the Fe−Sb bonds (1−3) and Sb−Sb bonds (4−6) in the $Sb_3Fe(CO)_2^-$ (C_s, $^1A'$) anion calculated at the B3LYP/SDD(Sb)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

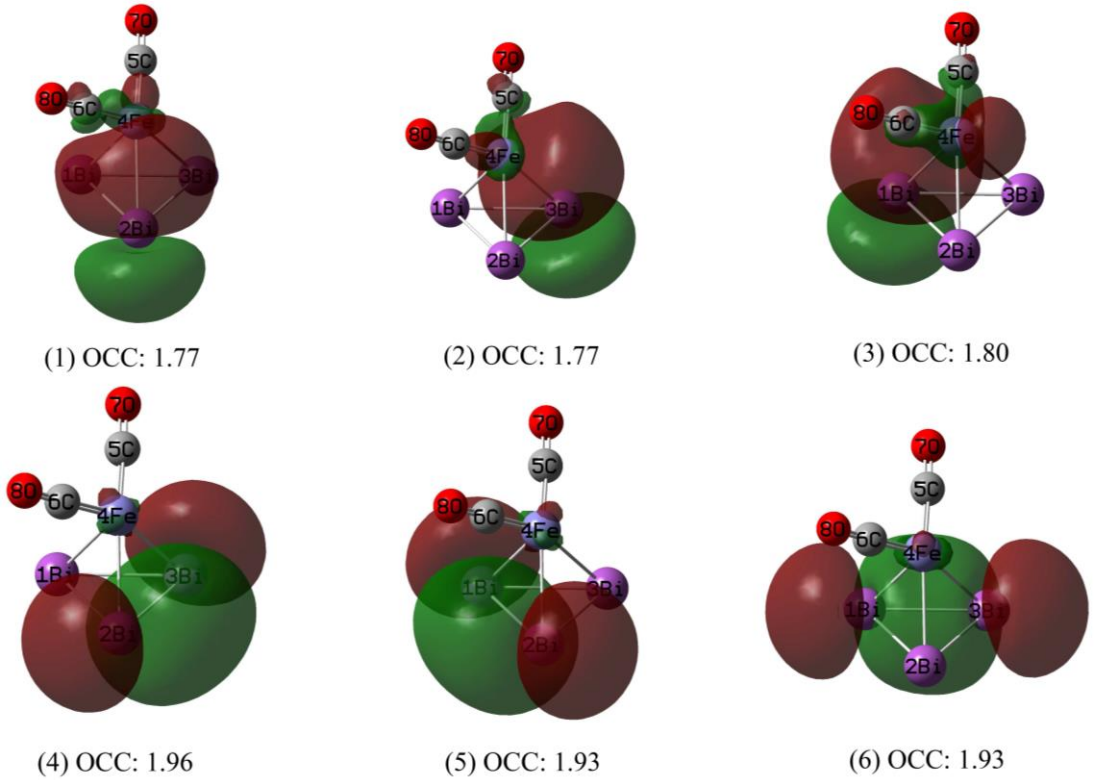

Fig. S10 Natural bonding orbitals related to the Fe−Bi bonds (1−3) and Bi−Bi bonds (4−6) in the $Bi_3Fe(CO)_2^-$ (C_s, $^1A'$) anion calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

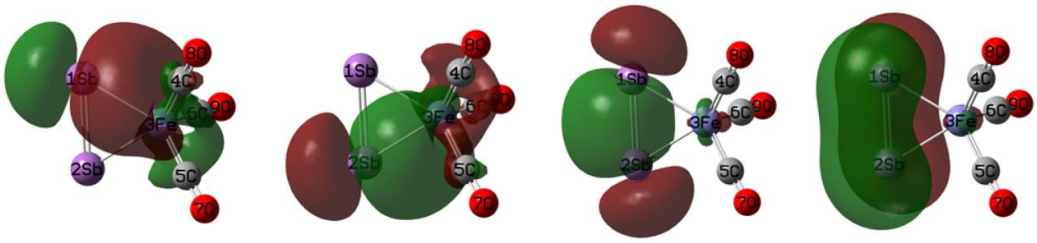

Fig. S11 Natural bonding orbitals related to the Fe−Sb bonds (1, 2) and Sb−Sb bonds (3, 4) in the $Sb_2Fe(CO)_3^-$ (C_s, $^2A'$) anion calculated at the B3LYP/SDD(Sb)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

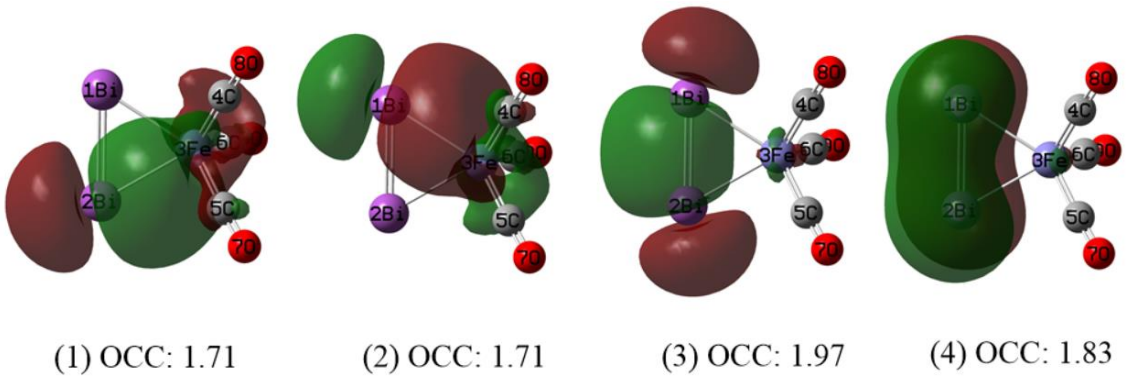

Fig. S12 Natural bonding orbitals related to the Fe−Bi bonds (1, 2) and Bi−Bi bonds (3, 4) in the $Bi_2Fe(CO)_3^-$ (C_s, $^2A'$) anion calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

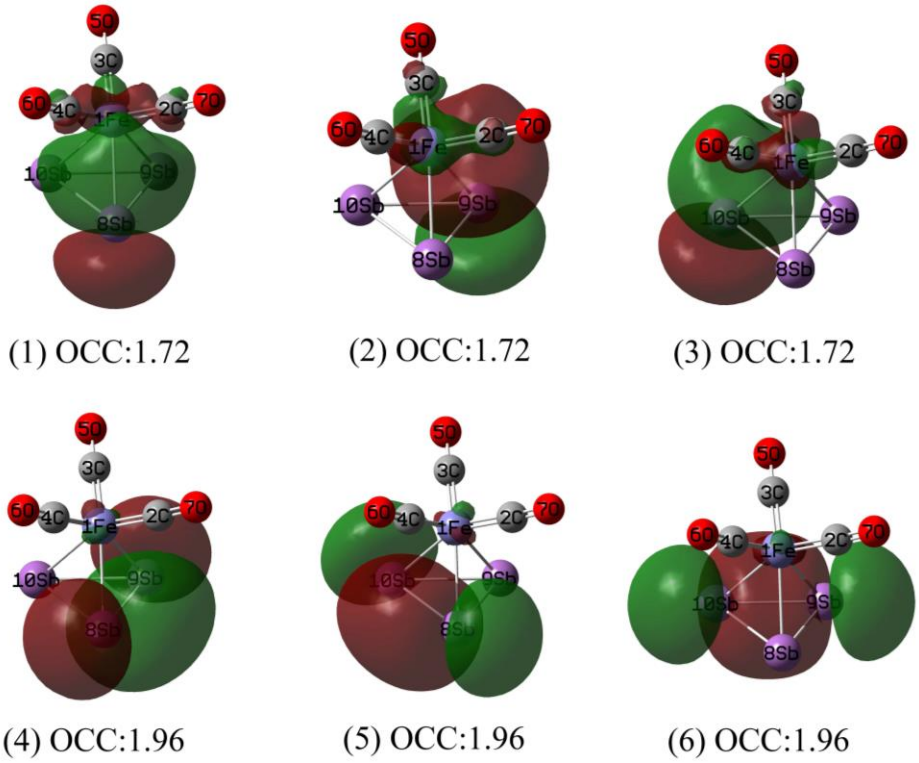

Fig. S13 Natural bonding orbitals related to the Fe−Sb bonds (1−3) and Sb−Sb bonds (4−6) in the $Sb_3Fe(CO)_3^-$ (C_{3v}, $^1A_1$) anion calculated at the B3LYP/SDD(Sb)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.

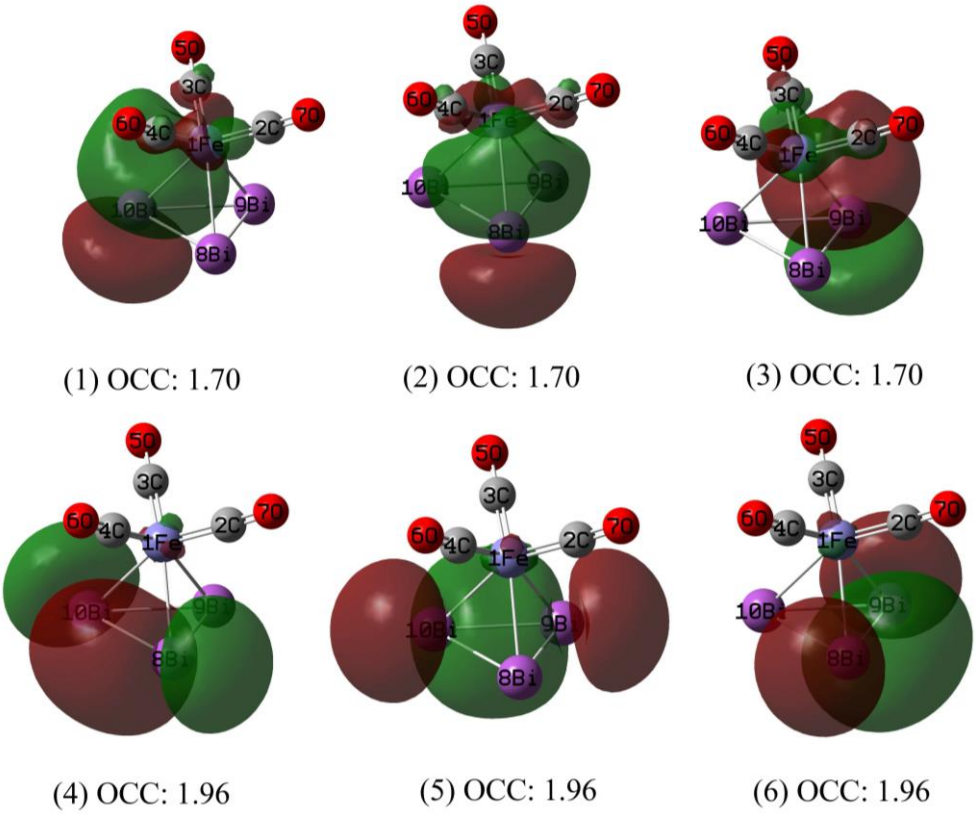

Fig. S14 Natural bonding orbitals related to the Fe−Bi bonds (1−3) and Bi−Bi bonds (4−6) in the $Bi_3Fe(CO)_3^-$ (C_{3v}, $^1A_1$) anion calculated at the B3LYP/SDD(Bi)/aug-cc-pVTZ(Fe, C, O) level of theory, with the total occupancy numbers listed below.